Access DB# 96160

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, RICHARD A. Examiner #: 78680 Date: FEB 25, 2005
Art Unit: 1713 Phone Number 272-1104 Serial Number: 10/723,350
Mail Box and Bldg/Room Location: REM 10A29 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

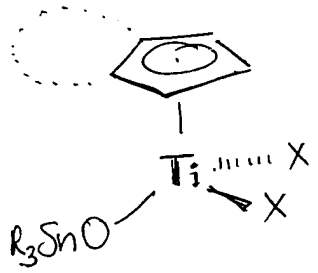
Title of Invention: STANNOXY-SUBSTITUTED METALLOCENE CATALYSTS

Inventors (please provide full names): MARTIN, Joel L. JENSEN, Michael D.
McDANIEL, Max P.

Earliest Priority Filing Date: 11-26-2003

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for compounds having the following minimum structure



- indenyl, cyclopentedienyl or fluorenyl π-ligand maybe substituted.
- R is alkyl, aryl (phenyl)
- key words which may help "monocyclo pentedienyl" "half sandwich" metallocene "half metallocene" "stannyl" "stannyloxy" "stannoxy"

STAFF USE ONLY

Searcher: EL
Searcher Phone #:
Searcher Location:
Date Searcher Picked Up:
Date Completed: 3-6-05
Searcher Prep & Review Time:
Clerical Prep Time:
Online Time:

Type of Search

NA Sequence (#)
AA Sequence (#)
Structure (#)
Bibliographic
Litigation
Fulltext
Patent Family
Other

Vendors and cost where applicable

STN
Dialog
Questel/Orbit
Dr.Link
Lexis/Nexis
Sequence Systems
WWW/Internet
Other (specify)

PTO-1590 (8-01)

CLAIMS

We Claim:

1. A compound having the following formula:

$(X^1)(X^2)(X^3)(X^4)M^1$; wherein

M^1 is selected from titanium, zirconium, or hafnium;

(X^1) is selected from cyclopentadienyl, indenyl, fluorenyl, substituted cyclopentadienyl, substituted indenyl, or substituted fluorenyl;

each substituent on the substituted cyclopentadienyl, substituted indenyl, or substituted fluorenyl (X^1) is independently selected from an aliphatic group, an aromatic group, a cyclic group, a combination of aliphatic and cyclic groups, an oxygen group, a sulfur group, a nitrogen group, a phosphorus group, an arsenic group, a carbon group, a silicon group, a germanium group, a tin group, a lead group, a boron group, an aluminum group, an inorganic group, an organometallic group, or a substituted derivative thereof, any one of which having from 1 to about 20 carbon atoms; a halide; or hydrogen;

(X^2) is selected from a stannoxy group with the following formula:

$-OSnR_3$;

wherein R is independently selected from alkyl, cycloalkyl, aryl, aralkyl, substituted alkyl, substituted aryl, or substituted aralkyl, any one of which having from 1 to about 20 carbon atoms; OR' wherein R' is selected from alkyl, aryl, aralkyl, substituted alkyl, substituted aryl, or substituted aralkyl, any one of which having from 1 to about 20 carbon atoms; F; Cl; Br; or I; and

(X^3) and (X^4) are independently selected from an aliphatic group, an aromatic group, a cyclic group, a combination of aliphatic and cyclic groups, an oxygen group, a sulfur group, a nitrogen group, a phosphorus group, an arsenic group, a carbon group, a silicon group, a germanium group, a tin group, a lead group, a boron group, an aluminum group, an inorganic group, an organometallic group, or a substituted derivative thereof, any one of which having from 1 to about 20 carbon atoms; or a halide.

2. The compound of Claim 1, wherein the compound has the following general formula:

$(\eta^5$-cycloalkadienyl$)M(OSnR_3)X_2$; wherein

cycloalkadienyl is selected from cyclopentadienyl, indenyl, fluorenyl, or substituted analogs thereof;

M is selected from Ti, Zr, or Hf;

R is independently selected from substituted or non-substituted alkyl, cycloalkyl, aryl, aralkyl, alkoxide, or aryloxide, any one of which having from 1 to about 20 carbon atoms; F; Cl; Br; or I; and

X is independently selected from F; Cl; Br; I; or a substituted or non-substituted alkyl, cycloalkyl, aryl, aralkyl, alkoxide, or aryloxide, any one of which having from 1 to about 20 carbon atoms.

3. The compound of Claim 1, wherein the compound is selected from:

$(\eta^5$-cyclopentadienyl)titanium(triphenylstannoxy)dichloride;

$(\eta^5$-cyclopentadienyl)zirconium(triphenylstannoxy)dichloride;

$(\eta^5$-cyclopentadienyl)titanium(trimethylstannoxy)dichloride;

$(\eta^5$-cyclopentadienyl)zirconium(triethylstannoxy)dichloride;

$(\eta^5$-cyclopentadienyl)hafnium(triphenylstannoxy)dichloride;

$(\eta^5$-cyclopentadienyl)titanium(tri-n-butylstannoxy)dichloride;

$(\eta^5$-cyclopentadienyl)titanium(triphenylstannoxy)dibromide;

$(\eta^5$-pentamethylcyclopentadienyl)titanium(triphenylstannoxy)dibromide;

or

$(\eta^5$-cyclopentadienyl)titanium(tributylstannoxy)dibromide.

4. A composition of matter comprising a half-sandwich metallocene compound with the following formula:

$(X^1)(X^2)(X^3)(X^4)M^1$; wherein

M^1 is selected from titanium, zirconium, or hafnium;

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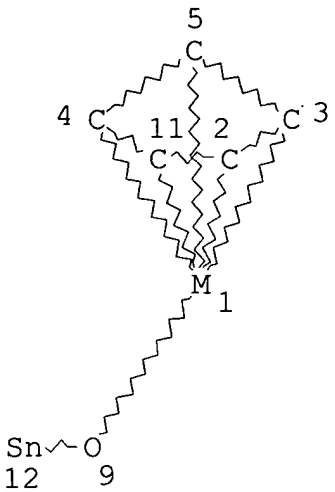

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L10 ANSWER 1 OF 3 ZCAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:721207 ZCAPLUS
DN 132:50061
ED Entered STN: 12 Nov 1999

TI Synthesis and X-ray crystal structure elucidation of an organometallic oxide containing Nb and Sn

AU Silva, Rosalice Mendonca; Huffmann, John C.
CS Departamento de Quimica, Universidade Federal de Minas Gerais, Belo Horizonte, 31270-901, Brazil

SO Polyhedron (1999), 18(22), 2823-2826
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
CC 29-8 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75

AB The organometallic oxide (.eta.5-C5H5)2Nb(Cl)(.mu.-O)Sn(Ph)2Cl2, 2, was prepd. and characterized by spectroscopic methods and elemental anal. The mol. structure was detd. by x-ray crystallog. The Nb atom is in a pseudotetrahedral coordination geometry environment comprised of the two Cp rings and the Cl and O atoms. The coordination geometry around the Sn atom is a distorted trigonal bipyramidal. The detd. Nb-O bond distance of 1.789(6) .ANG. indicates a partial double bonding between Nb and O. Although the Sn-O bond can be described as a dative bond, it is a very strong interaction, 2.22(16) .ANG.. The formation of 2 involved the activation of one of the Sn-Cphenyl bonds of the Sn starting material. Residual H2O present in the reaction solvent was the source of the bridging O in the mol.

ST crystal structure niobium tin oxide complex; mol structure niobium tin oxide; niobium tin oxide complex prepn structure

IT Crystal structure
Molecular structure
(of a niobium-tin oxide complex)

IT **252990-49-1P**
(crystal structure; prepn. and structure of a niobium-tin oxide complex)

IT 639-58-7, Chlorotriphenylstannane 12793-14-5, Niobocene dichloride
(prepn. and structure of a niobium-tin oxide complex)

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(2) Chisholm, M; Inorg Chem 1984, V23, P1021 ZCAPLUS
(3) Eaborn, C; J Chem Soc Dalton Trans 1976, P767 ZCAPLUS
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(6) Holt, M; Chem Rev 1989, V89, P11 ZCAPLUS
(7) Labinger, J; Adv Chem Ser 1979, V167, P149
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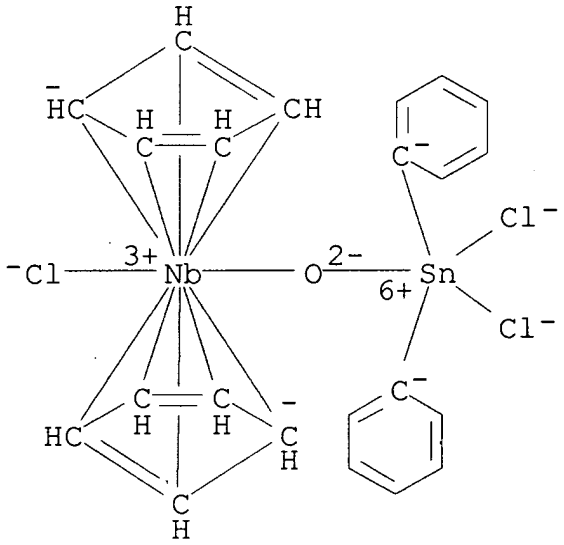
(10) Okara, R; J Organomet Chem 1964, V1, P356
(11) Prout, K; Acta Crystallogr Sect B 1974, V30, P2290

(12) Rheingold, A; Acta Crystallogr Sect C 1991, V47, P1963
(13) Silva, R; PhD Thesis Universidade Federal de Minas Gerais 1989
(14) Skripkin, Y; J Coord Chem 1985, V3, P570
(15) Steunou, N; Inorg Chem 1998, V37, P910
(16) Urbanos, F; J Organomet Chem 1984, V276, P185 ZCAPLUS

IT **252990-49-1P**
(crystal structure; prepn. and structure of a niobium-tin oxide complex)

RN 252990-49-1 ZCAPLUS

CN Niobium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(dichlorodiphenyltin)-.mu.-oxo-, stereoisomer (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:634252 ZCAPLUS
DN 129:316333
ED Entered STN: 08 Oct 1998
TI Formation of sulfido niobium complexes through C-S bond activation
AU Azevedo, Nelio Pires; Lopes, Antonio Ricardo Giuliani; Silva, Rosalice Mendonca; Speziali, Nivaldo Lucio; Abras, Anuar; Horner, Manfredo; Burrow, Robert Alan
CS Departmento de Quimica, Universidade Federal de Minas Gerais, Belo Horizonte, 31.270-901, Brazil
SO Journal of the Brazilian Chemical Society (1998), 9(3), 279-285
CODEN: JOCSET; ISSN: 0103-5053
PB Sociedade Brasileira de Quimica
DT Journal
LA English

CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75

AB Upon reacting (.eta.5-C5H5)2NbCl2, .eta.5-C5H5 = Cp, and (Ph)3Sn(SPh), in THF, [(.eta.5-C5H5)2Nb(Cl)(.mu.-S)Sn(Ph)3(Cl)] (1) and (.eta.5-C5H5)2Nb(S)Cl (2) were obtained. Complexes 1 and 2 were characterized by IR, 1H-NMR, 13C-NMR, Mossbauer spectroscopies, elemental anal. as well as by at. absorption. Hydrolysis of 1 yielded the .mu.-oxo species, [(.eta.5-C5H5)2Nb(Cl)(.mu.-O)Sn(Ph)3Cl], which was characterized by IR, 1H-NMR, 13C-NMR and Mossbauer spectroscopies, elemental anal., at. absorption as well as by x-ray crystallog. It crystallizes in the space group Pca21 with a 17.282(3), b 18.122(4), c 17.3269(2) , and Z = 8. Addnl. studies indicated that the complexes were formed as a result of the nucleophilic displacement of the Nb-chloride bond by the thiolate ligand followed by a C-S bond cleavage. The cleavage occurs with an excess of the thiolate compd. equal to or >2:1.

ST crystal structure niobium tin oxo bridged; mol structure niobium tin oxo bridged; niobium sulfido complex prepn hydrolysis; tin niobium oxo bridged prepn structure; carbon sulfur bond activation phenylthiostannane niobium

IT Bond cleavage
(carbon-sulfur; of (phenylthio)triphenylstannane in reactions with niobium chloro cyclopentadienyl complex)

IT Reduction, electrochemical
Reduction potential
(of niobium cyclopentadienyl sulfido and niobium-tin cyclopentadienyl sulfido-bridged complexes)

IT Crystal structure
Molecular structure
(of niobium-tin cyclopentadienyl chloro Ph oxo-bridged dinuclear complex)

IT 1441-22-1, Triphenyl(phenylthio)stannane 12793-14-5, Dichlorobis(.eta.5-cyclopentadienyl)niobium
(carbon-sulfur bond cleavage in reaction of niobium chloro cyclopentadienyl complex with triphenyl(phenylthio)stannane)

IT 139-66-2, Diphenyl sulfide 1064-10-4, Hexaphenyldistannane
(formation from niobium chloro cyclopentadienyl complex with triphenyl(phenylthio)stannane)

IT **214785-34-9P**
(prepn. and crystal structure of)

IT 214785-32-7P, Chlorobis(.eta.5-cyclopentadienyl)(thio)niobium
(prepn. and electrochem. of)

IT 214785-31-6P
(prepn., electrochem. and hydrolysis of)

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(4) Boorman, P; Inorg Chem 1991, V30, P3886 ZCAPLUS
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(18) Kawaguchi, H; Organometallics 1997, V16, P307 ZCAPLUS
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(29) Rheingold, A; Acta Cryst 1991, VC47, P1963 ZCAPLUS
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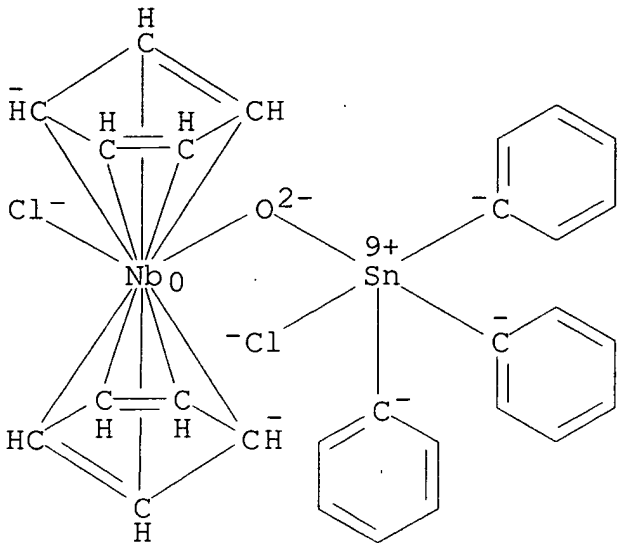
(32) Urbanos, F; J Organomet Chem 1984, V276, P185 ZCAPLUS
(33) Wilkinson, G; J Chem Soc, Dalton Trans 1980, P1888

IT **214785-34-9P**
(prepn. and crystal structure of)

RN 214785-34-9 ZCAPLUS

CN Niobium, chloro(chlorotriphenyltin)bis(.eta.5-2,4-cyclopentadien-1-yl)-.mu.-oxo-, stereoisomer (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:574309 ZCAPLUS
DN 111:174309
ED Entered STN: 10 Nov 1989
TI Multiple bonds between Main Group elements and transition metals. LXV. Addition of hexamethyldistannane to an organometal oxide with cleavage of the tin-tin bond
AU Herrmann, Wolfgang A.; Marz, Dieter W.
CS Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.
SO Journal of Organometallic Chemistry (1989), 362(1-2), C5-C7
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA German
CC 29-11 (Organometallic and Organometalloidal Compounds)
OS CASREACT 111:174309
AB A general synthetic route to trialkylstannoxy compds. of the organotransition metal series was found, viz. the addn. of Me2SnSnMe3 to trioxo(.eta.5-pentamethylcyclopentadienyl)rhenium(VII) . The reaction occurs with concomitant cleavage of the tin-tin bond, and the air-sensitive product oxo(.eta.5-pentamethylcyclopentadienyl)bis(trimethylstannoxy)rhenium(V) (I) was obtained in 90% yield. The Bu deriv. of I is prepd. analogously.
ST hexamethyldistannane addn trioxopentamethylcyclopentadienylrhenium; rhenium pentamethylcyclopentadienyl trioxide addn hexaalkyldistannane; stannoxypentamethylcyclopentadienylrhenium oxide; oxopentamethylcyclopentadienylbistrialkylstannoxyrhenium; tin tin bond cleavage hexaalkyldistannane; stannoxyrhenium oxo

cyclopentadienyl

IT Addition reaction
(of hexaalkyldistannanes with trioxo(pentamethylcyclopentadienyl) rhenium)

IT Bond cleavage
(tin-tin, in addn. reaction of trioxo(pentamethylcyclopentadienyl)rhenium with hexaalkyldistannanes)

IT 90695-83-3
(addn. reaction of, with hexamethyl- and hexabutyldistannane)

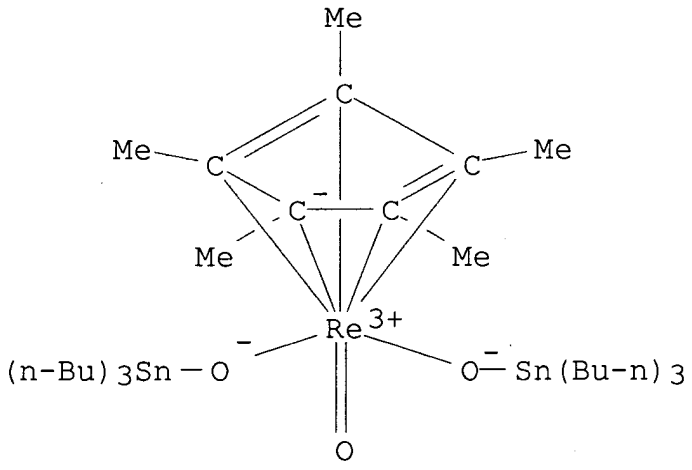
IT 661-69-8, Hexamethyldistannane 813-19-4, Hexabutyldistannane
(addn. reaction of, with trioxo(pentamethylcyclopentadienyl)rheni um, tin-tin bond cleavage by)

IT **123037-83-2P 123060-03-7P**
(prepn. of)

IT **123037-83-2P 123060-03-7P**
(prepn. of)

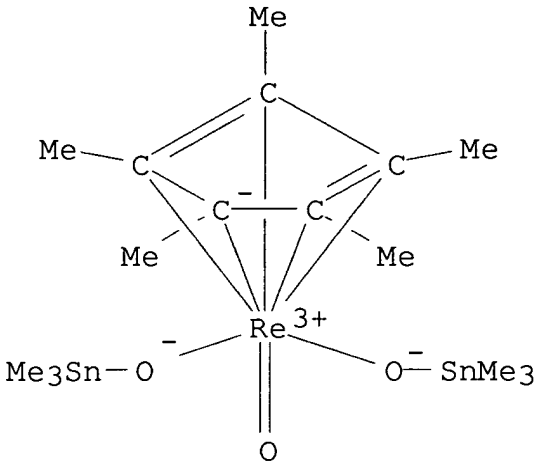
RN 123037-83-2 ZCAPLUS

CN Rhenium, oxo[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]bis(tributylhydroxystannanato)- (9CI) (CA INDEX NAME)



RN 123060-03-7 ZCAPLUS

CN Rhenium, bis(hydroxytrimethylstannanato)oxo[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)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